

Geometrical phase for a three-dimensional anisotropic quantum well

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Abstract

A three-dimensional anisotropic quantum well placed in an adiabatically precessing uniform magnetic field is considered and an explicit formula for the Berry phase is obtained. To get the Berry phase, a purely algebraic algorithm of reducing a quadratic Hamiltonian to the canonical form via symplectic transformations of the phase space is presented.

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I. INTRODUCTION

In the classical work [1], M.Berry has shown that if an evolution of a physical system is cyclic and adiabatic the geometric phase (so-called Berry phase) is accumulated on the wave function in addition to the usual dynamical phase. The Berry phase has a purely geometric nature and reflects geometric properties of the parameter space of the system. B.Simon [2] has given an interpretation of the Berry phase as due to holonomy in a line bundle over the parameter space.

The space of values of the magnetic induction as a parameter space for the considered system is frequently dealt with. As a rule, for a magnetic field, the Berry phase is studied in the two cases: (1) a potential well is transported along a closed loop in the usual configuration space [3, 4, 5]; (2) spin particles interact with a time-dependend magnetic field [6, 7, 8]. The most part of theoretical studies is devoted to the evolution of the spin in a magnetic field; in this case explicit formulae are easy to obtain using finite-dimensional algebra. However, the Berry phase can arise in the case of a spin-less particle interacting with a precessing magnetic field [9].

The aim of this paper is to obtain an explicit formula for the Berry phase in the case of a three-dimensional anisotropic quantum well placed in a precessing magnetic field. The classical Hamiltonian of such a system is a quadratic form of momenta and positions. The considered problem has attracted attention of physicists since the 1980's. In particular, M.Berry [10] has calculated the geometric phase for a one-dimensional quadratic potential with variable coefficients. As for now, the most general result for quadratic Hamiltonians is contained in [9] where the following simple case has been studied: a quadratic potential has an axial symmetry with respect to the z -axis and a magnetic field precesses around z -axis. These assumptions reduce the dimension of the problem and significantly simplify calculations. We investigate the most general problem in the case in which the frequencies of the parabolic potential are mutually different and the magnetic field is arbitrarily directed.

The significant peculiarity of a quadratic quantum Hamiltonian lies in the fact that the Feynman integrals for their propagators can be calculated explicitly. What is more, the problem of calculating these integrals is reduced to finding the canonical form for a classical counterpart of the Hamiltonian via symplectic transformations of the phase space; in our case this form is a sum of squares of momenta and positions). Finding the canonical form is a standard (but as a rule very cumbersome) problem of linear algebra. For convenience of readers, in the next section we present an algorithm of finding the classical (symplectic) and quantum (unitary) transformations that reduce the corresponding Hamiltonian to the canonical form.

It is important to stress that we obtain our results using only simple methods of linear algebra. It is strange enough that in the similar situations, more complicated methods are used in the physical literature; in particular, the method of the Bogolubov canonical transformations [11] or other indirect methods. Note another advantage of the method we use. To find various physical quantities one needs the matrix elements of the corresponding operators. However, a direct calculation of matrix elements can be a complicated problem. Our method allows to resolve this problem using only simple calculations from linear algebra. As an example we can mention the papers [12] and [13] where the hybrid and hybrid-phonon resonances for an asymmetric quantum well in a magnetic field have been studied by means of this approach.

II. PRELIMINARIES

The advantage of a description of mechanical systems with the help of the Hamilton formalism is conditioned by the following main reason: a choice of the generalized coordinates is restricted by no conditions (any one of quantities defining the state of a system may be the generalized coordinates.) What is more it is possible to choose such a class of transformations of phase coordinates that includes the transformation of the all initial phase coordinates p_i, q_i to the new ones P_i, Q_i (here $i = 1, 2, \dots, n$; n is the dimension of the configuration space) because momenta and positions play the same role in Hamilton equations

$$Q = Q(p, q); P = P(p, q). \quad (1)$$

However there is a restriction. The transformation (1) is permissible (canonical) if and only if it conserves the Poisson brackets. The equivalent criterion for the transformation (1) to be canonical is the equality to the exact differential the 1-form $pdq - PdQ$. This 1-form is the exact differential of the generating function of the canonical transformation (1).

$$dS = pdq - PdQ. \quad (2)$$

Note that if we know the generating function we can always find the functions determining the transformation (1).

Through the paper we use the notation

$$[x_1|x_2] = -\langle p_1|q_2 \rangle + \langle p_2|q_1 \rangle \quad (3)$$

for the standard symplectic product in the phase space $\mathbb{R}^{2n} = \mathbb{R}_q^n \times \mathbb{R}_p^n$; here $x_j = (p_j, q_j)$, ($j = 1, 2$).

Recall that a linear transformation

$$\begin{pmatrix} p \\ q \end{pmatrix} = L \begin{pmatrix} P \\ Q \end{pmatrix}. \quad (4)$$

is canonical (i.e., preserves the Poisson brackets) if and only if the matrix L is symplectic:

$$[Lx_1|Lx_2] \equiv [x_1|x_2]. \quad (5)$$

It is convenient to write the matrix L in the form

$$\begin{pmatrix} L_1 & L_2 \\ L_3 & L_4 \end{pmatrix}. \quad (6)$$

The following commutation relations between components of the matrix L follow immediately from the fact that the matrix L is symplectic

$$L_1^*L_4 - L_2^*L_3 = E, \quad L_3^*L_4 - L_4^*L_3 = 0, \quad L_1^*L_2 - L_2^*L_1 = 0, \quad (7)$$

where E is the unit matrix.

Denote by S the generating function for the transformation L (this means by definition that $dS = pdq - PdQ$); we will suppose that S is a function of p and P . Then

$$Q = -\frac{\partial S(p, P)}{\partial P}, \quad q = \frac{\partial S(p, P)}{\partial p}. \quad (8)$$

In this case the generating function of the canonical transformation (4) is expressed in terms of L_i by the following formula (we assume that $|L_2| \neq 0$)

$$S(p, P) = -\langle P|L_2^{-1}p\rangle + \frac{1}{2}\langle P|L_2^{-1}L_1P\rangle + \frac{1}{2}\langle p|L_4L_2^{-1}p\rangle. \quad (9)$$

According to the Dirac-Fock theorem [14] the classical transformation (4) corresponds to a quantum transformation $U : L^2(\mathbb{R}_p^n) \rightarrow L^2(\mathbb{R}_p^n)$ that is to a unitary operator related to L as follows

$$\begin{aligned} U^{-1}\hat{p}U &= L_1\hat{P} + L_2\hat{Q}, \\ U^{-1}\hat{q}U &= L_3\hat{P} + L_4\hat{Q}. \end{aligned} \quad (10)$$

The operator U can be represented as an integral operator

$$(Uf)(p) = \int U(p, P)f(P)dP. \quad (11)$$

with the kernel

$$U(p, P) = C \exp \left[-\frac{i}{\hbar} S(p, P) \right], \quad (12)$$

where the normalization constant $C = ((2\pi\hbar)^3 |\det L_2|)^{-1/2}$. Then using the unitarity of the operator U we can express the initial wave function of the quantum Hamiltonian in terms of the final wave functions by the following formula

$$\psi(p) = C \int \tilde{\psi}(P) \exp \left[-\frac{i}{\hbar} S(p, P) \right] dP, \quad (13)$$

here $\psi(p)$ is the wave function of the original Hamiltonian and $\tilde{\psi}(P)$ is the wave function of the unitary equivalent Hamiltonian.

III. DIAGONALIZATION OF QUADRATIC HAMILTONIANS

The purpose of this section is to demonstrate an algorithm of reducing the quadratic Hamiltonian

$$H(p, q) = \frac{1}{2} \begin{pmatrix} p \\ q \end{pmatrix} \tilde{H} \begin{pmatrix} p \\ q \end{pmatrix}, \quad (14)$$

where \tilde{H} is a symmetric matrix of order $2n \times 2n$, to the canonical form. This form must contain only squares of the corresponding momenta and positions.

Then Hamilton equations corresponding to our quadratic Hamiltonian (14) can be written in the form $\dot{x} = I\tilde{H}x$, here I is the symplectic unity

$$I = \begin{pmatrix} 0 & -E \\ E & 0 \end{pmatrix}. \quad (15)$$

At first we find the family $(\lambda_i)_{1 \leq i \leq 2n}$ of eigenvalues the matrix $I\tilde{H}$, where I is the symplectic unity

$$I = \begin{pmatrix} 0 & -E \\ E & 0 \end{pmatrix}, \quad (16)$$

and the family $(f_i)_{1 \leq i \leq 2n}$ of the corresponding eigenvectors. For this purpose we use the following simple lemma

Lemma. *The characteristic polynomial $\det(I\tilde{H} - \lambda E)$ has only real coefficients and contains only terms of even degree.*

It follows from the Lemma that if λ_i is an eigenvalue of the matrix $I\tilde{H}$ then $-\lambda_i$ and λ_i^* are eigenvalues of this matrix too. Taking into account this assertion we can arrange λ_i in a finite sequence of the form

$$\nu_1, \dots, \nu_l, i\omega_1, \dots, i\omega_m, -\nu_1, \dots, -\nu_l, -i\omega_1, \dots, -i\omega_m, \quad (17)$$

where $\nu_i, \omega_k > 0$; $l, m \geq 0$; $l + m = n$.

Now we transform the basis (f_i) into a symplectic one. Let $(b_i)_{1 \leq i \leq 2n}$ be the following sequence of vectors from \mathbf{R}^{2n} :

$$f_1(\nu_1), \dots, f_l(\nu_l), \operatorname{Re}[f_1(i\omega_1)], \dots, \operatorname{Re}[f_m(i\omega_m)], f_1(-\nu_1), \dots, f_l(-\nu_l), \operatorname{Im}[f_1(i\omega_1)], \dots, \operatorname{Im}[f_m(i\omega_m)]. \quad (18)$$

It is clear that the vectors $(b_i)_{1 \leq i \leq 2n}$ form a basis of the space \mathbf{R}^{2n} . These vectors satisfy the skew-orthogonality conditions

$$\begin{cases} [b_i | b_k] = 0, & \text{if } i < k; \quad i + n \neq k, \\ [b_i | b_{i+n}] \neq 0, & \forall i = 1, \dots, n. \end{cases} \quad (19)$$

Denote $c_i = [b_i | b_{i+n}]$, then according to (19) the vectors b'_i ,

$$\begin{cases} b'_i = -\frac{\operatorname{sgn}(c_i)}{\sqrt{|c_i|}} b_i; & i = 1, \dots, n, \\ b'_{i+n} = \frac{1}{\sqrt{|c_i|}} b_{i+n}; & i = 1, \dots, n, \end{cases} \quad (20)$$

form a symplectic basis of the space \mathbf{R}^{2n} . Using coordinates with respect to this basis, we reduce the Hamiltonian H to the form

$$H = -2 \sum_{i=1}^l \nu_i P_i Q_i + \sum_{i=1}^m \varepsilon_i \omega_i (P_{i+l}^2 + Q_{i+l}^2), \quad (21)$$

where $\varepsilon_i = \operatorname{sgn} c_i$.

Now we define the canonical basis of the quadratic form \tilde{H} by the relations

$$\begin{cases} a_i = b'_i, & \text{if } l+1 \leq i \leq n \text{ and } n+l+1 \leq i \leq 2n, \\ a_i = -\frac{1}{\sqrt{2}}(b'_i + b'_{i+n}), & \text{if } 1 \leq i \leq l, \\ a_{i+n} = \frac{1}{\sqrt{2}}(b'_i - b'_{i+n}), & \text{if } 1 \leq i \leq l. \end{cases} \quad (22)$$

With respect to this basis, the Hamiltonian H has the canonical form

$$H(P, Q) = \sum_{i=1}^l \nu_i (P_i^2 - Q_i^2) + \sum_{i=1}^m \varepsilon_i \omega_i (P_{i+l}^2 + Q_{i+l}^2). \quad (23)$$

The transition matrix from the initial phase coordinates p, q to the final ones P, Q can be written in the following form

$$L = [a_1, a_2, a_3, a_4, a_5, a_6], \quad (24)$$

where each vector a_i is written in the corresponding column.

IV. DIAGONALIZATION OF THE HAMILTONIAN OF A 3D ANISOTROPIC OSCILLATOR WITH A MAGNETIC FIELD

Let us consider the Hamiltonian of a 3D anisotropic harmonic oscillator with a magnetic field \mathbf{B} arbitrarily directed with respect to the potential symmetry axes

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{m}{2} (\Omega_x^2 x^2 + \Omega_y^2 y^2 + \Omega_z^2 z^2). \quad (25)$$

Here \mathbf{A} is the vector potential of the magnetic field, c is the light velocity, Ω_i ($i = x, y, z$) are the characteristic frequencies of the parabolic potential, m , e , and \mathbf{p} are the mass, the charge, and the momentum of the considered particle.

The results of Sec. III show that Hamiltonian (25) is unitary equivalent to a quadratic Hamiltonian without magnetic field but with new frequencies named "hybrid frequencies". The purpose of this section is to reduce Hamiltonian (25) to the canonical form

$$H(\mathbf{P}, \mathbf{Q}) = \frac{1}{2m} (P_1^2 + P_2^2 + P_3^2) + \frac{m}{2} (\omega_1^2 Q_1^2 + \omega_2^2 Q_2^2 + \omega_3^2 Q_3^2), \quad (26)$$

using the algorithm developed in the preceding section; here \mathbf{P}, \mathbf{Q} are the new phase coordinates, ω_i ($i = 1, 2, 3$) are the hybrid frequencies. It is convenient to choose the following gauge for the vector potential \mathbf{A}

$$\mathbf{A} = \left(\frac{1}{2} B_y z - B_z y, 0, B_x y - \frac{1}{2} B_y x \right). \quad (27)$$

Below we use the notations

$$K_1^2 = m^2 \Omega_x^2, \quad K_2^2 = m^2 \Omega_y^2, \quad K_3^2 = m^2 \Omega_z^2;$$

$$p_x = p_1, \quad p_y = p_2, \quad p_z = p_3; \quad x = q_1, \quad y = q_2, \quad z = q_3;$$

$$\frac{eB_x}{2c} = B_1, \quad \frac{eB_y}{2c} = B_2, \quad \frac{eB_z}{2c} = B_3.$$

In this notation

$$H = \frac{1}{2m} [(p_1 - B_2 q_3 + 2B_3 q_2)^2 + p_2^2 + (p_3 + B_2 q_1 - 2B_1 q_2)^2 + K_1^2 q_1^2 + K_2^2 q_2^2 + K_3^2 q_3^2], \quad (28)$$

i.e., H is a quadratic form of p and q with the matrix

$$\tilde{H} = \frac{1}{m} \begin{pmatrix} 1 & 0 & 0 & 0 & 2B_3 & -B_2 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & B_2 & -2B_1 & 0 \\ 0 & 0 & B_2 & \bar{K}_1 & -2B_1 B_2 & 0 \\ 2B_3 & 0 & -2B_1 & -2B_1 B_2 & \bar{K}_2 & -2B_2 B_3 \\ -B_2 & 0 & 0 & 0 & -2B_2 B_3 & \bar{K}_3 \end{pmatrix}, \quad (29)$$

where $\bar{K}_1 = K_1^2 + B_2^2$, $\bar{K}_2 = K_2^2 + 4B_1^2 + 4B_3^2$, $\bar{K}_3 = K_3^2 + B_2^2$.

To find the eigenvalues of the matrix $I\tilde{H}$ we solve the equation $\det(I\tilde{H} - \lambda E) = 0$, which is easily reduced to the form

$$\begin{vmatrix} 1 & 0 & 0 & -\mu & 2B_3 & -B_2 \\ 0 & 1 & 0 & 0 & -\mu & 0 \\ 0 & 0 & 1 & B_2 & -2B_1 & -\mu \\ 0 & 0 & 0 & K_1^2 + \mu^2 & -2B_3\mu & 2B_2\mu \\ 0 & 0 & 0 & 2B_3\mu & K_2^2 + \mu^2 & -2B_1\mu \\ 0 & 0 & 0 & -2B_2\mu & 2B_1\mu & K_3^2 + \mu^2 \end{vmatrix} = 0, \quad (30)$$

where $\mu = m\lambda$. Since

$$\det \begin{pmatrix} A & B \\ 0 & C \end{pmatrix} = \det(AC) \quad (31)$$

for any $n \times n$ matrix A, B, C , we can obtain the hybrid frequencies from the following sixth-order algebraic equation [15]

$$(\Omega_x^2 + \lambda^2)(\Omega_y^2 + \lambda^2)(\Omega_z^2 + \lambda^2) + \omega_{xc}^2(\Omega_x^2 + \lambda^2)\lambda^2 + \omega_{yc}^2(\Omega_y^2 + \lambda^2)\lambda^2 + \omega_{zc}^2(\Omega_z^2 + \lambda^2)\lambda^2 = 0, \quad (32)$$

where $\omega_{ic} = eB_i/mc$ are the components of the cyclotron frequency and $\lambda_i^\pm = \pm i\omega_i$. Note that equation (32) always has three different real negative solutions with respect to λ^2 .

Now our purpose is to find the eigenvectors of the matrix $I\tilde{H}$ associated with the eigenvalues λ_i^\pm . Using elementary matrix transformations one can reduce the matrix $M = I\tilde{H} - \lambda E$ to the form

$$M = \frac{1}{m} \begin{pmatrix} 0 & 0 & 0 & -K_1^2 - \mu^2 & 2B_3\mu & -B_2\mu \\ 0 & 0 & 0 & -2B_3\mu & -K_2^2 - \mu^2 & 2B_1\mu \\ 0 & 0 & 0 & 2B_2\mu & -2B_1\mu & -K_3^2 - \mu^2 \\ 1 & 0 & 0 & -\mu & 2B_3 & -B_2 \\ 0 & 1 & 0 & 0 & -\mu & 0 \\ 0 & 0 & 1 & B_2 & -2B_1 & -\mu \end{pmatrix} \equiv \frac{1}{m} \begin{pmatrix} 0 & X \\ E & Y \end{pmatrix}. \quad (33)$$

The eigenvectors of (33) are obtained from the system

$$\begin{cases} X\mathbf{q} = 0, \\ \mathbf{p} = -Y\mathbf{q}. \end{cases} \quad (34)$$

Solving this system we get the coordinates of the eigenvectors $g(\mu)$ associated with the eigen-

values $\mu = m\lambda_i^\pm$ of $I\tilde{H}$:

$$\begin{aligned}
p_1 &= -2B_3K_1^2(K_3^2 + \mu^2) - 4B_2^2B_3\mu^2 - 2B_1B_2\mu(K_1^2 - \mu^2), \\
p_2 &= \mu(K_1^2 + \mu^2)(K_3^2 + \mu^2) + 4B_2^2\mu^3, \\
p_3 &= 2B_1K_3^2(K_1^2 + \mu^2) + 4B_1B_2\mu^2 - 2B_2B_3\mu(K_3^2 - \mu^2). \\
q_1 &= 2B_3\mu(K_3^2 + \mu^2) + 4B_1B_2\mu^2, \\
q_2 &= (K_1^2 + \mu^2)(K_3^2 + \mu^2) + 4B_2^2\mu^2, \\
q_3 &= 4B_2B_3\mu^2 - 2\mu B_1(K_1^2 + \mu^2).
\end{aligned} \tag{35}$$

Consider the vectors

$$\begin{aligned}
f_1 &= \text{Re } [g(-im\omega_1)], \quad f_2 = \text{Re } [g(-im\omega_2)], \quad f_3 = \text{Re } [g(-im\omega_3)], \\
f_4 &= \text{Im } [g(-im\omega_1)], \quad f_5 = \text{Im } [g(-im\omega_2)], \quad f_6 = \text{Im } [g(-im\omega_3)].
\end{aligned}$$

Then we have for the coordinates of f_i the following expressions. If $i = 1, 2, 3$, then

$$\text{Rep}_1 = -2B_3K_1^2(K_3^2 - m^2\omega_i^2) + 4B_2^2B_3m^2\omega_i^2, \quad \text{Rep}_2 = 0,$$

$$\text{Rep}_3 = 2B_1K_3^2(K_1^2 - m^2\omega_i^2) - 4B_1B_2^2m^2\omega_i^2,$$

$$\text{Req}_1 = -4B_1B_2m^2\omega_i^2, \quad \text{Req}_2 = (K_1^2 - m^2\omega_i^2)(K_3^2 - m^2\omega_i^2) - 4B_2^2m^2\omega_i^2, \quad \text{Req}_3 = -4B_2B_3m^2\omega_i^2.$$

If $i = 4, 5, 6$, then

$$\text{Imp}_1 = 2B_1B_2m\omega_{i-3}(K_1^2 + m^2\omega_{i-3}^2), \quad \text{Imp}_2 = -m\omega_{i-3}(K_1^2 - m^2\omega_{i-3}^2)(K_3^2 - m^2\omega_{i-3}^2) + 4B_2^2m^3\omega_{i-3}^3,$$

$$\text{Imp}_3 = -2B_2B_3m\omega_{i-3}(K_3^2 + m^2\omega_{i-3}^2),$$

$$\text{Imq}_1 = -2B_3m\omega_{i-3}(K_3^2 - m^2\omega_{i-3}^2), \quad \text{Imq}_2 = 0, \quad \text{Imq}_3 = 2m\omega_{i-3}B_1(K_1^2 - m^2\omega_{i-3}^2).$$

Denote

$$\begin{aligned}
M_i &= m^4 \{ \omega_{yc}^2 \omega_i^4 (\omega_{xc}^2 + \omega_{yc}^2) + \omega_{xc}^2 \Omega_z^2 (\Omega_x^2 - \omega_i^2)^2 + \omega_{zc}^2 \Omega_x^2 (\Omega_z^2 - \omega_i^2)^2 + \\
&\quad + [(\Omega_x^2 - \omega_i^2)(\Omega_z^2 - \omega_i^2) - \omega_{yc}^2 \omega_i^2]^2 \}^{1/2}
\end{aligned} \tag{36}$$

for $i = 1, 2, 3$; and $M_i = M_{i-3}$ for $i = 4, 5, 6$. It is easy to show that the following basis is symplectic

$$h_i = \frac{1}{M_i \sqrt{m\omega_i}} f_i, \tag{37}$$

where we put $\omega_i = \omega_{i-3}$ for $i = 4, 5, 6$.

With respect to this basis the Hamiltonian H has the form

$$H = \frac{1}{2} \sum_{i=1}^3 \omega_i (\tilde{p}_i^2 + \tilde{q}_i^2), \tag{38}$$

here \tilde{p}_i , and \tilde{q}_i are new phase coordinates.

To reduce this Hamiltonian to the canonical form (26) we change the variables once again

$$P_i = \sqrt{m\omega_i}\tilde{p}_i; \quad Q_i = \frac{1}{\sqrt{m\omega_i}}\tilde{q}_i. \quad (39)$$

Finally, the transition matrix L from the initial coordinates to the coordinates P_i, Q_i has the components

$$l_{ij} = \frac{a_{ij}}{M_i \sqrt{m\omega_i}}, \quad (40)$$

where a_{ij} are defined as follows:

if $i = 1, 2, 3$ then

$$\begin{aligned} a_{i1} &= -m^5 \omega_{zc} \Omega_x^2 (\Omega_z^2 - \omega_i^2) + \frac{1}{2} m^5 \omega_{zc} \omega_{yc}^2 \omega_i^2, \quad a_{i2} = 0, \quad a_{i3} = m^5 \omega_{xc} \Omega_z^2 (\Omega_x^2 - \omega_i^2) - \frac{1}{2} m^5 \omega_{xc} \omega_{yc}^2 \omega_i^2, \\ a_{i4} &= -m^4 \omega_{xc} \omega_{yc} \omega_i^2, \quad a_{i5} = m^4 (\Omega_x^2 - \omega_i^2) (\Omega_z^2 - \omega_i^2) - m^4 \omega_{yc}^2 \omega_i^2, \quad a_{i6} = -m^4 \omega_{yc} \omega_{zc} \omega_i^2; \end{aligned}$$

if $i = 4, 5, 6$ then

$$\begin{aligned} a_{i1} &= \frac{1}{2} m^5 \omega_{xc} \omega_{yc} \omega_{i-3} (\Omega_x^2 + \omega_{i-3}^2), \quad a_{i2} = -m^5 \omega_{i-3} (\Omega_x^2 - \omega_{i-3}^2) (\Omega_z^2 - \omega_{i-3}^2) + m^5 \omega_{yc}^2 \omega_{i-3}^3, \\ a_{i3} &= \frac{1}{2} m^5 \omega_{yc} \omega_{zc} \omega_{i-3} (\Omega_z^2 + \omega_{i-3}^2), \quad a_{i4} = -m^4 \omega_{zc} \omega_{i-3} (\Omega_z^2 - \omega_{i-3}^2), \\ a_{i5} &= 0, \quad a_{i6} = m^4 \omega_{xc} \omega_{i-3} (\Omega_x^2 - \omega_{i-3}^2). \end{aligned}$$

As a result we have obtained an explicit formula for the transition matrix L .

Note that the quantum counterpart of classical Hamiltonian (21) is the quantum harmonic oscillator with the eigenvalues

$$E_{n_1 n_2 n_3} = \hbar \omega_1 \left(n_1 + \frac{1}{2} \right) + \hbar \omega_2 \left(n_2 + \frac{1}{2} \right) + \hbar \omega_3 \left(n_3 + \frac{1}{2} \right), \quad (41)$$

where $n_1, n_2, n_3 = 0, 1, \dots$. In the P -representation, the corresponding eigenfunctions are

$$\tilde{\psi}_n(\mathbf{P}) = (\omega_1 \omega_2 \omega_3)^{-1/4} \chi_{n_1} \left(\frac{P_1}{\sqrt{\omega_1 \hbar}} \right) \chi_{n_2} \left(\frac{P_2}{\sqrt{\omega_2 \hbar}} \right) \chi_{n_3} \left(\frac{P_3}{\sqrt{\omega_3 \hbar}} \right). \quad (42)$$

Here χ_n is the n -th oscillator function

$$\chi_n(x) = (\pi^{1/2} 2^n n!)^{-1/2} \exp(-x^2/2) H_n(x),$$

where H_n is the corresponding Hermite polynomial.

V. CALCULATING THE BERRY PHASE

The purpose of this section is to obtain an explicit formula for the Berry phase of a 3D anisotropic parabolic quantum well placed in a precessing magnetic field. We deal with the case when a considered quantum state undergoes an adiabatic evolution in the space of the values of the magnetic induction \mathbf{B} in such a way that eigenvalues (41) remain nondegenerate. Let $\psi_{\mathbf{n}}$ be the wave function of the original state (here $\mathbf{n} = (n_1, n_2, n_3)$ is the set of the quantum numbers). If the system undergoes an evolution in question, then the wave function obtains the geometric phase

$$\gamma_{\mathbf{n}} = \oint_C \mathbf{V}_{\mathbf{n}}(\mathbf{B}) d\mathbf{B}, \quad (43)$$

where C is a closed path $\mathbf{B}(t)$ in the parameter space such that $\mathbf{B}(T) = \mathbf{B}(0)$, and $\mathbf{V}_{\mathbf{n}}(\mathbf{B})$ is so-called Berry vector potential given by

$$\mathbf{V}_{\mathbf{n}}(\mathbf{B}) = i\langle\psi_{\mathbf{n}}(\mathbf{B})|\nabla_{\mathbf{B}}\psi_{\mathbf{n}}(\mathbf{B})\rangle = -\text{Im}\langle\psi_{\mathbf{n}}(\mathbf{B})|\nabla_{\mathbf{B}}\psi_{\mathbf{n}}(\mathbf{B})\rangle. \quad (44)$$

Since the Berry phase is determined by $\mathbf{V}_{\mathbf{n}}(\mathbf{B})$, it is sufficient to calculate only the vector potential. In our case the magnetic field doesn't vanish and hence the parameter space is $\mathbf{R}^3 \setminus \{0\}$, which is topologically non-trivial, and we can expect that the Berry phase is non-trivial, too.

To find the scalar product in (44) one needs eigenfunctions of the initial Hamiltonian. However, a direct calculation of the wave functions to obtain the Berry phase is a complicated computational problem. To calculate the Berry phase, we suggest to simplify the calculations using the method of linear canonical transformation of the phase space developed in the preceding sections. In this case we can use formula (11) to express the initial wave functions $\psi_{\mathbf{n}}(\mathbf{P}; \mathbf{B})$ in terms of the final ones (42):

$$\psi_{\mathbf{n}}(\mathbf{p}; \mathbf{B}) = C \int \tilde{\psi}_{\mathbf{n}}(\mathbf{P}; \mathbf{B}) \exp \left[-\frac{i}{\hbar} S(\mathbf{p}, \mathbf{P}) \right] d\mathbf{P}. \quad (45)$$

Taking into account that $\tilde{\psi}_{\mathbf{n}}(\mathbf{P}; \mathbf{B})$ is real-valued we can calculate $\nabla_{\mathbf{B}}\psi_{\mathbf{n}}(\mathbf{p}; \mathbf{B})$:

$$\begin{aligned} \nabla_{\mathbf{B}}\psi_{\mathbf{n}}(\mathbf{p}; \mathbf{B}) &= \int \left[\nabla_{\mathbf{B}} C \tilde{\psi}_{\mathbf{n}}(\mathbf{P}; \mathbf{B}) \right] \exp \left[-\frac{i}{\hbar} S(\mathbf{p}, \mathbf{B}) \right] d\mathbf{P} - \\ &\quad - \frac{i}{\hbar} \int C \tilde{\psi}_{\mathbf{n}}(\mathbf{P}; \mathbf{B}) \exp \left[-\frac{i}{\hbar} S(\mathbf{p}, \mathbf{P}) \right] [\nabla_{\mathbf{B}} S(\mathbf{p}, \mathbf{P})] d\mathbf{P}. \end{aligned} \quad (46)$$

In what follows we denote $\nabla_{\mathbf{B}}$ simply by ∇ .

Let us calculate scalar product (44)

$$\langle\psi_{\mathbf{n}}|\nabla\psi_{\mathbf{n}}\rangle = \int d\mathbf{p} \psi_{\mathbf{n}}^*(\mathbf{p}) \nabla\psi_{\mathbf{n}}(\mathbf{p}) = \int d\mathbf{p} \left\{ C^* \int \int d\mathbf{P} d\mathbf{P}' \tilde{\psi}_{\mathbf{n}}(\mathbf{P}') \left[\nabla C \tilde{\psi}_{\mathbf{n}}(\mathbf{P}) \right] \times \right.$$

$$\begin{aligned}
& \times \exp \left[\frac{i}{\hbar} (S(\mathbf{p}, \mathbf{P}') - S(\mathbf{p}, \mathbf{P})) \right] - \frac{i}{\hbar} \int \int d\mathbf{P} d\mathbf{P}' |C|^2 \tilde{\psi}_{\mathbf{n}}(\mathbf{P}') \tilde{\psi}_{\mathbf{n}}(\mathbf{P}) \times \\
& \times \exp \left[\frac{i}{\hbar} (S(\mathbf{p}, \mathbf{P}') - S(\mathbf{p}, \mathbf{P})) \right] \nabla S(\mathbf{p}, \mathbf{P}) \Big\}. \tag{47}
\end{aligned}$$

By changing the variables $L_2^{-1} \mathbf{p} / \hbar = \mathbf{y}$; $d\mathbf{p} = |\det L_2| \hbar^3 d\mathbf{y}$, we perform the integration with respect to \mathbf{p} in the first term of (47) and get

$$\begin{aligned}
& \int \exp \left[\frac{i}{\hbar} (S(\mathbf{p}, \mathbf{P}') - S(\mathbf{p}, \mathbf{P})) \right] d\mathbf{p} = \\
& = \exp \left[\frac{i}{2\hbar} (\langle \mathbf{P}' | L_2^{-1} L_1 \mathbf{P}' \rangle - \langle \mathbf{P} | L_2^{-1} L_1 \mathbf{P} \rangle) \right] |\det L_2| \hbar^3 \int \exp [i \langle \mathbf{P} - \mathbf{P}' | \mathbf{y} \rangle] d\mathbf{y} = \\
& = (2\pi \hbar)^3 |\det L_2| \delta(\mathbf{P} - \mathbf{P}'). \tag{48}
\end{aligned}$$

Hence the first term in (47) is real-valued and doesn't contribute in the Berry phase. Therefore, we need to calculate only the second term in (47).

It is convenient to introduce the notations

$$A = -\nabla L_2^{-1}; \quad B = \frac{1}{2} \nabla (L_2^{-1} L_1); \quad D = \frac{1}{2} \nabla (L_4 L_2^{-1}); \quad \Lambda = \frac{1}{2\hbar} (\langle \mathbf{P}' | L_2^{-1} L_1 \mathbf{P}' \rangle - \langle \mathbf{P} | L_2^{-1} L_1 \mathbf{P} \rangle). \tag{49}$$

Now integrating the second term in (47) with respect to \mathbf{p} , we obtain

$$\begin{aligned}
I &= \int \exp \left[\frac{i}{\hbar} (S(\mathbf{p}, \mathbf{P}') - S(\mathbf{p}, \mathbf{P})) \right] \nabla S(\mathbf{p}, \mathbf{P}) d\mathbf{p} = \\
& \hbar^3 |\det L_2| \exp(i\Lambda) \times \\
& \left[(2\pi)^3 \langle \mathbf{P} | B \mathbf{P} \delta(\mathbf{P} - \mathbf{P}') \rangle - i\hbar (2\pi)^3 \sum_{k=1}^3 [(AL_2)^* \mathbf{P}]_k \partial_k \delta(\mathbf{P} - \mathbf{P}') - \right. \\
& \left. \hbar^2 (2\pi)^3 (\langle \partial | L_2^* D L_2 \partial \rangle) \delta(\mathbf{P} - \mathbf{P}') \right]. \tag{50}
\end{aligned}$$

Calculating the corresponding derivatives

$$\partial_k \exp(i\Lambda) = -\frac{i}{\hbar} [(L_2^{-1} L_1 \mathbf{P})_k] \exp(i\Lambda), \tag{51}$$

$$\partial_l \partial_k \exp(i\Lambda) = -\frac{i}{\hbar} (L_2^{-1} L_1)_{kl} \exp(i\Lambda) - \frac{i}{\hbar} (L_2^{-1} L_1 \mathbf{P})_k (L_2^{-1} L_1 \mathbf{P})_l \exp(i\Lambda), \tag{52}$$

and substituting (51) and (52) into (50) after simple algebra we get, taking away the imaginary part,

$$\text{Re} I =$$

$$(2\pi\hbar)^3 |\det L_2| \left\{ \langle \mathbf{P}' | B \mathbf{P}' \rangle + \langle \mathbf{P}' | A L_1 \mathbf{P}' \rangle + \langle \mathbf{P}' | L_1^* D L_1 \mathbf{P}' \rangle - \hbar^2 \langle \partial | L_2^* D L_2 \partial \rangle \right\} \delta(\mathbf{P} - \mathbf{P}'). \quad (53)$$

As a result we have the following formula for the Berry vector potential

$$\begin{aligned} \mathbf{V}_n(\mathbf{B}) = & -\text{Im} \int d\mathbf{p} \psi_n^*(\mathbf{p}) \nabla \psi_n(\mathbf{p}) = \frac{1}{\hbar} \int \int d\mathbf{P} d\mathbf{P}' |C|^2 \tilde{\psi}_n(\mathbf{P}') \psi_n(\mathbf{P}) (\text{Re} I) = \\ & \frac{1}{\hbar} (2\pi\hbar)^3 |\det L_2| |C|^2 \left\{ \int d\mathbf{P}' [\langle \mathbf{P}' | B \mathbf{P}' \rangle + \langle \mathbf{P}' | (A L_1) \mathbf{P}' \rangle + \langle \mathbf{P}' | (L_1^* D L_1) \mathbf{P}' \rangle] |\tilde{\psi}_n(\mathbf{P}')|^2 + \right. \\ & \left. \hbar^2 \int d\mathbf{P} d\mathbf{P}' \sum_{k,l=1}^3 (L_2^* D L_2) \partial_l \partial_k \delta(\mathbf{P} - \mathbf{P}') \tilde{\psi}_n(\mathbf{P}') \tilde{\psi}_n(\mathbf{P}) \right\}. \end{aligned} \quad (54)$$

Denote

$$\begin{cases} F = B + A L_1 + L_1^* D L_1, \\ G = L_2^* D L_2. \end{cases} \quad (55)$$

It is clear that $G^* = G$ and we can rewrite (54) in the form

$$\begin{aligned} \mathbf{V}_n(\mathbf{B}) = & \frac{1}{\hbar} (2\pi\hbar)^3 |\det L_2| |C|^2 \left\{ \int d\mathbf{P}' \langle \mathbf{P}' | F \mathbf{P}' \rangle |\tilde{\psi}_n(\mathbf{P}')|^2 d\mathbf{P}' + \right. \\ & \left. \hbar^2 \int d\mathbf{P} d\mathbf{P}' \sum_{k,l=1}^3 G_{lk} \partial_l \partial_k \delta(\mathbf{P} - \mathbf{P}') \tilde{\psi}_n(\mathbf{P}') \tilde{\psi}_n(\mathbf{P}) \right\}. \end{aligned} \quad (56)$$

Using (42), we get

$$\int P_k P_l |\tilde{\psi}_n(\mathbf{P})|^2 d\mathbf{P} = 0,$$

if $k \neq l$, and

$$\int P_k^2 |\tilde{\psi}_n(\mathbf{P})|^2 d\mathbf{P} = \omega_k \hbar \int \chi_{n_k}^2(q) q^2 dq = \left(n_k + \frac{1}{2} \right) \hbar \omega_k.$$

Since

$$\int \chi_n(x) \chi_n'(x) dx = 0, \quad (57)$$

it follows for $k \neq l$

$$\int \tilde{\psi}_n(\mathbf{P}) \partial_k \partial_l \tilde{\psi}_n(\mathbf{P}) d\mathbf{P} = 0. \quad (58)$$

If $k = l$, then

$$\int \tilde{\psi}_n(\mathbf{P}) \partial_k^2 \tilde{\psi}_n(\mathbf{P}) d\mathbf{P} = -\frac{1}{\omega_k \hbar} \left(n_k + \frac{1}{2} \right). \quad (59)$$

Finally we have

$$\mathbf{V}_n(\mathbf{B}) = \sum_{k=1}^3 \left(n_k + \frac{1}{2} \right) \left[\omega_k F_{kk} + \frac{G_{kk}}{\omega_k} \right]. \quad (60)$$

Equation (60) is the main result of our paper. This formula extends a result of Berry [10] to the 3D case and contains as a particular case some results from [9].

Remark. Note that Formula (60) is valid in more general situations. Namely, let $H(\xi)$ be a family of quadratic Hamiltonians in the state space $L^2(\mathbb{R}^3)$ depending on a parameter ξ , $\xi \in X$, where the parameter space X is a smooth manifold. Let $\xi = \xi(t)$ be a curve in X such that $H(\xi(t))$ has three different eigenvalues at each t . Then the Berry phase corresponding to an adiabatic evolution along the curve $\xi = \xi(t)$ is given by (60), if we replace $\nabla_{\mathbf{B}}$ by ∇_{ξ} in all the auxiliary expressions.

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